

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
 Data File : VN084862.D
 Acq On : 14 Nov 2024 19:22
 Operator : JC\MD
 Sample : P4770-02 500X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-3

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
 Title : SW846 8260

Signal : TIC: VN084862.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	52	58	67	rVB4	6310	13284	1.39%	0.140%
2	2.824	140	148	149	rBV5	8087	15943	1.66%	0.168%
3	2.895	152	160	161	rBV6	10004	20102	2.10%	0.212%
4	7.224	889	896	905	rBV2	4418	12471	1.30%	0.131%
5	7.441	924	933	942	rVB2	3421	10039	1.05%	0.106%
6	8.159	1045	1055	1060	rBV	134418	326759	34.10%	3.444%
7	8.218	1060	1065	1075	rVB	246457	542025	56.57%	5.712%
8	8.577	1116	1126	1134	rBV	145805	344604	35.96%	3.632%
9	8.753	1145	1156	1179	rVB5	31185	172683	18.02%	1.820%
10	9.100	1206	1215	1224	rBV	350470	728016	75.98%	7.672%
11	10.006	1364	1369	1376	rBV3	5673	11077	1.16%	0.117%
12	10.147	1387	1393	1398	rVB4	8302	16698	1.74%	0.176%
13	10.565	1455	1464	1469	rBV	499632	941148	98.22%	9.918%
14	10.629	1469	1475	1486	rVB	516153	954121	99.58%	10.055%
15	11.865	1677	1685	1694	rBV	475384	849126	88.62%	8.949%
16	11.959	1694	1701	1711	rVV	124454	209585	21.87%	2.209%
17	12.065	1711	1719	1731	rVB	352615	655829	68.44%	6.912%
18	12.394	1768	1775	1785	rVB	143588	246664	25.74%	2.600%
19	12.688	1817	1825	1832	rBV2	35316	57999	6.05%	0.611%
20	12.847	1844	1852	1862	rBV	410829	696877	72.73%	7.344%
21	13.035	1875	1884	1888	rBV	44776	75606	7.89%	0.797%
22	13.094	1888	1894	1898	rVV	142351	246331	25.71%	2.596%
23	13.129	1898	1900	1903	rVV	66841	82126	8.57%	0.865%
24	13.170	1903	1907	1914	rVB	83004	133253	13.91%	1.404%
25	13.335	1928	1935	1941	rVB	59300	97275	10.15%	1.025%
26	13.482	1953	1960	1968	rBV	279695	463291	48.35%	4.882%
27	13.606	1974	1981	1987	rBV7	4140	9814	1.02%	0.103%
28	13.676	1987	1993	1999	rVB5	5240	10454	1.09%	0.110%
29	13.788	2005	2012	2026	rBV2	501214	958185	100.00%	10.098%
30	13.947	2035	2039	2040	rBV	9434	10596	1.11%	0.112%
31	13.988	2040	2046	2062	rVB3	57357	199084	20.78%	2.098%
32	14.182	2073	2079	2084	rVB3	10121	15328	1.60%	0.162%
33	14.235	2084	2088	2092	rVV4	17013	30402	3.17%	0.320%
34	14.270	2092	2094	2099	rVV	17137	20560	2.15%	0.217%
35	14.329	2099	2104	2110	rVB	32048	48218	5.03%	0.508%
36	14.441	2119	2123	2130	rVB3	9958	17641	1.84%	0.186%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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37	14.564	2138	2144	2153	rVB4	7312	12976	1.35%	0.137%
38	14.647	2153	2158	2162	rBV	18799	32138	3.35%	0.339%
39	14.688	2162	2165	2171	rVB	27978	36940	3.86%	0.389%
40	14.917	2201	2204	2211	rBV4	12293	21294	2.22%	0.224%
41	15.047	2215	2226	2231	rBV5	21483	55835	5.83%	0.588%
42	15.311	2267	2271	2282	rVB4	5235	12633	1.32%	0.133%
43	15.641	2315	2327	2333	rBV2	29535	58043	6.06%	0.612%
44	16.776	2514	2520	2522	rBV3	9098	15815	1.65%	0.167%

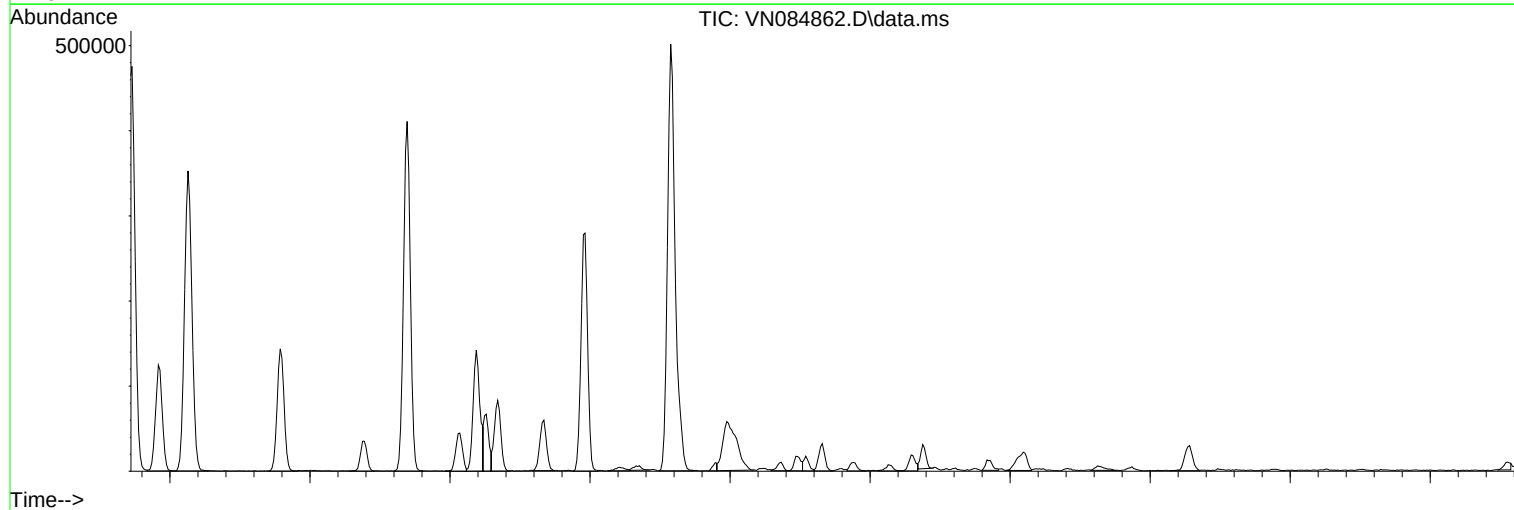
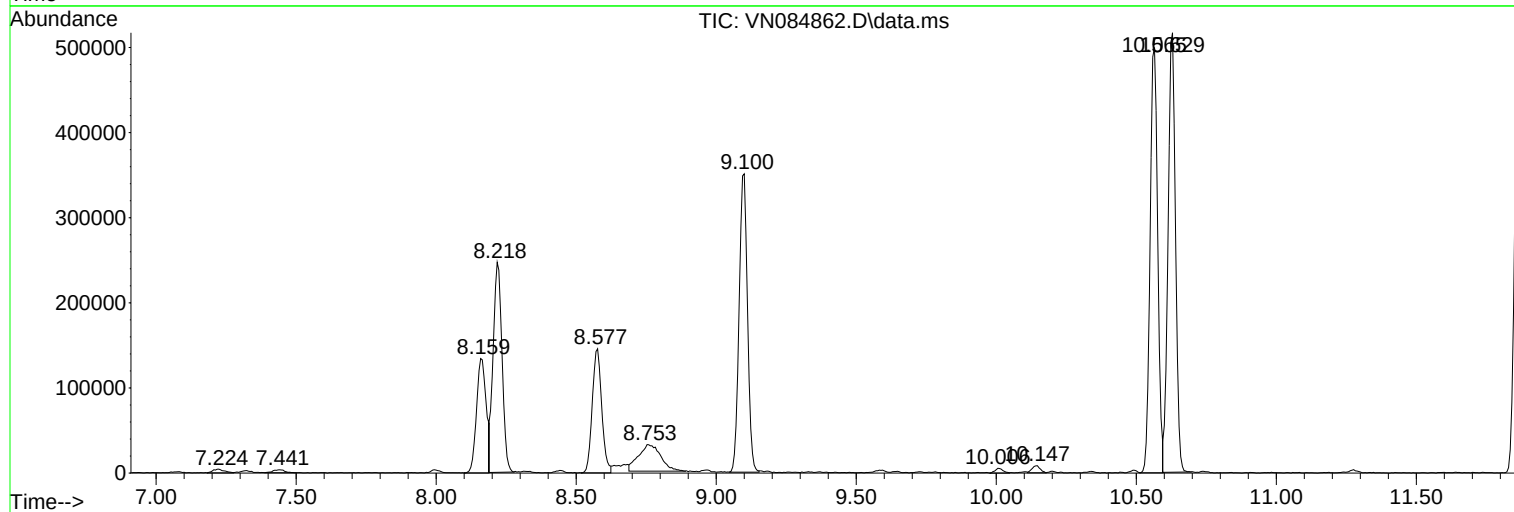
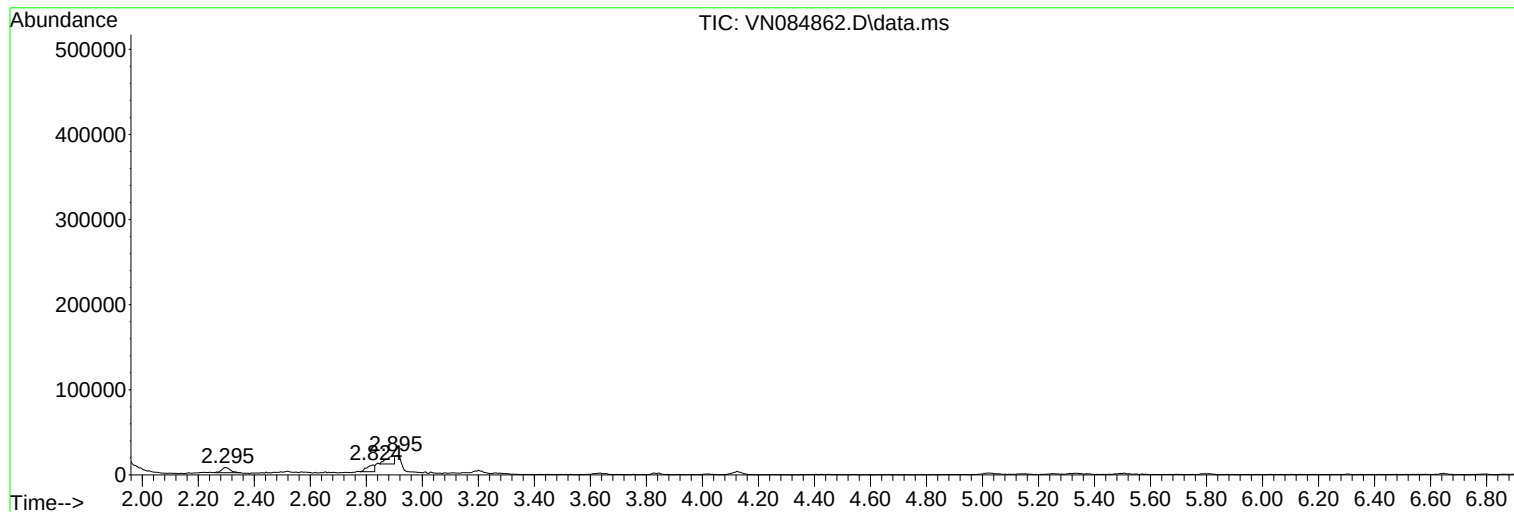
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
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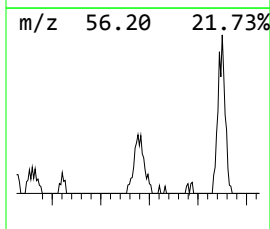
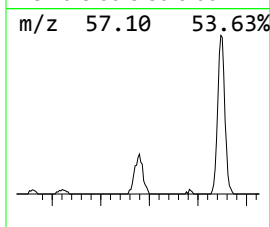
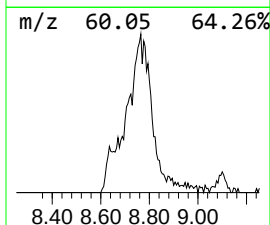
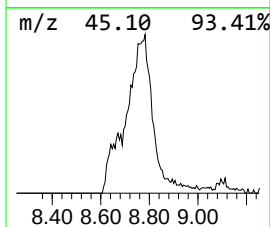
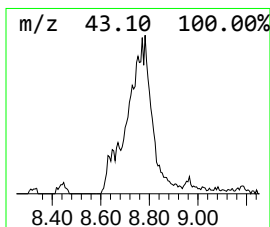
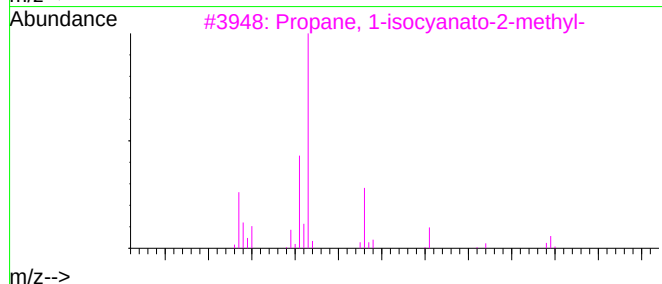
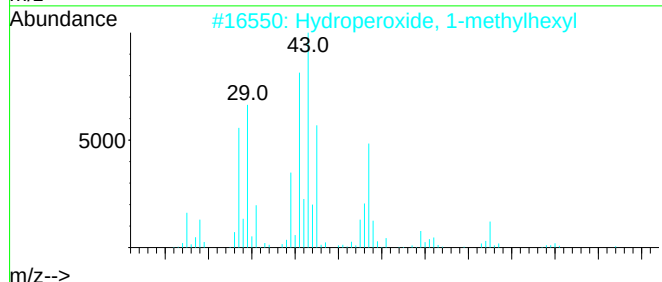
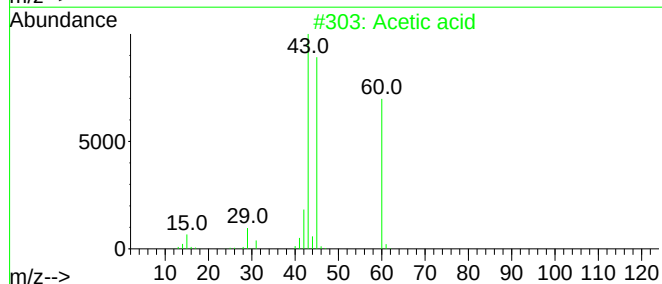
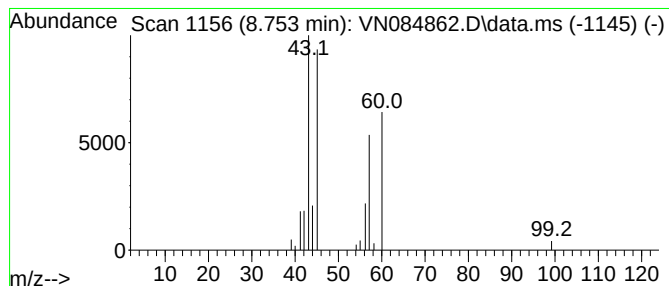
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.753	11.86 ug/l	172683	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	53
2	Hydroperoxide, 1-methylhexyl	132	C7H16O2	000762-46-9	25
3	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	14
4	1-Cyclopropylguanidine	99	C4H9N3	168627-33-6	10
5	1-Butaneboronic acid	102	C4H11BO2	004426-47-5	9



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

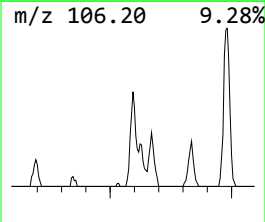
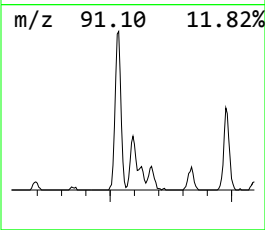
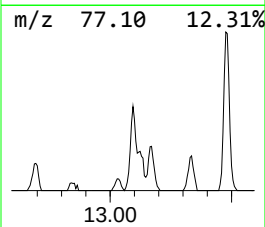
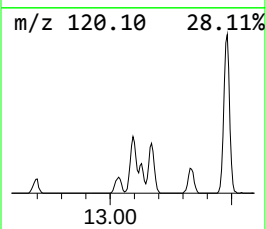
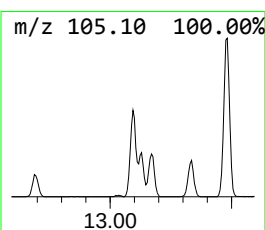
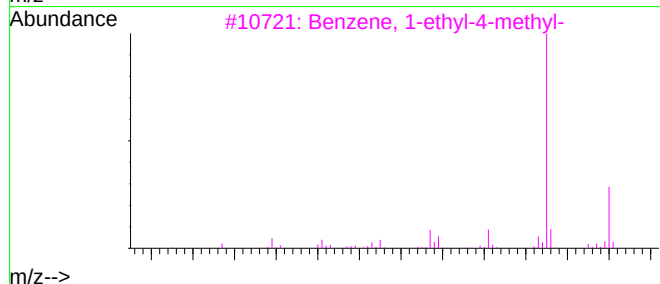
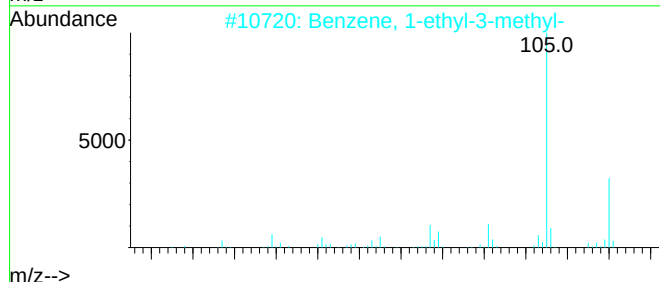
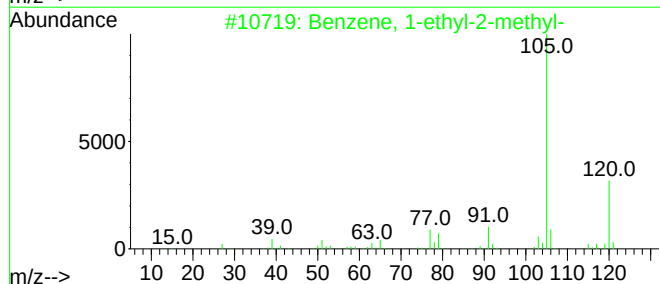
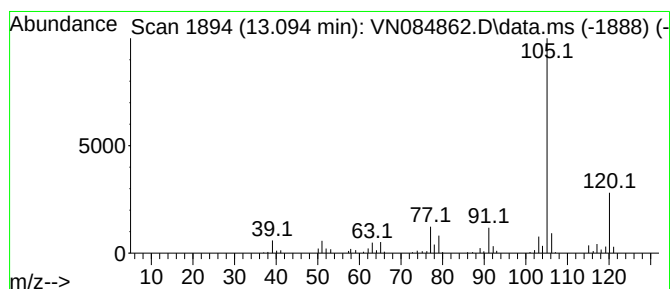
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	12.85 ug/l	246331	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

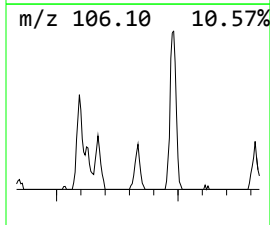
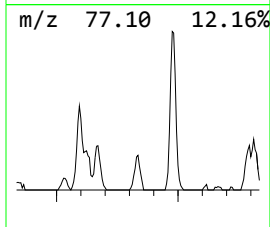
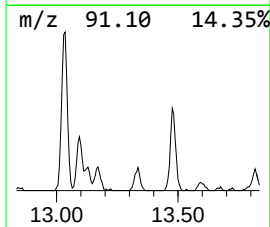
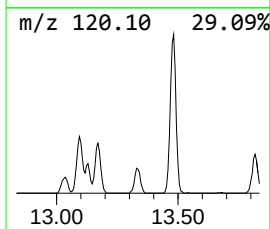
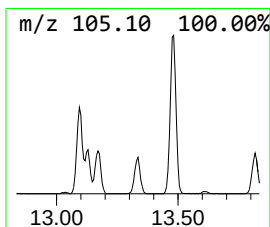
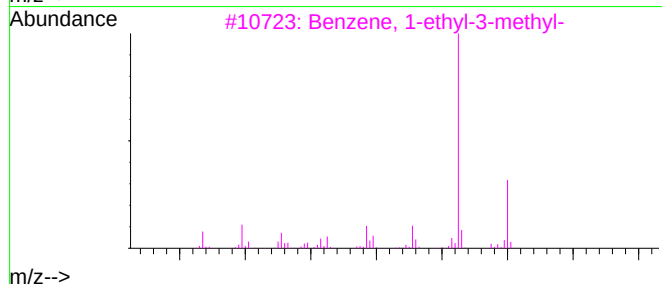
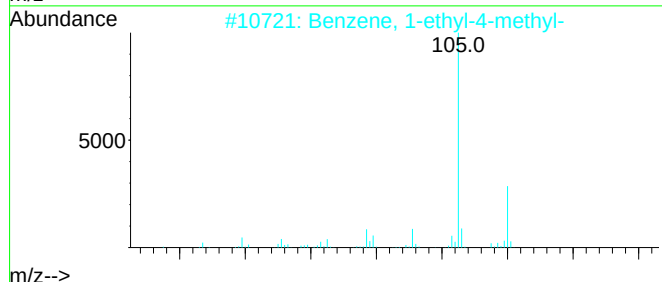
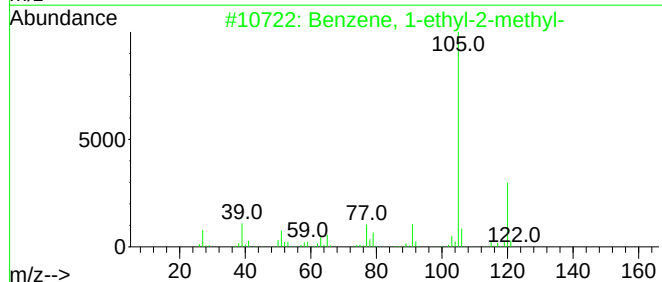
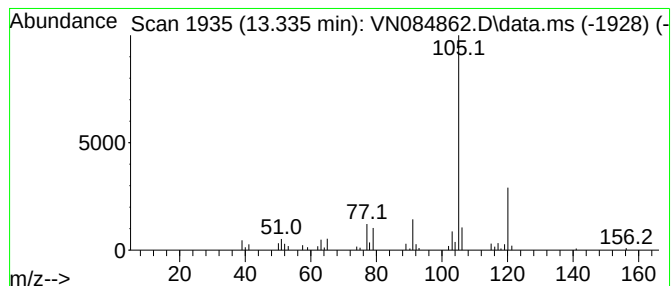
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	5.08 ug/l	97275	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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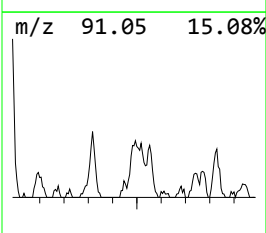
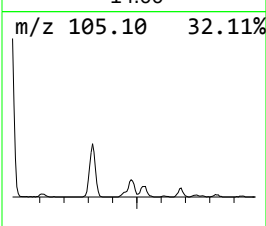
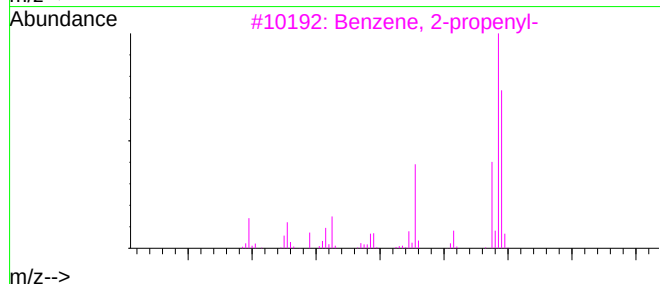
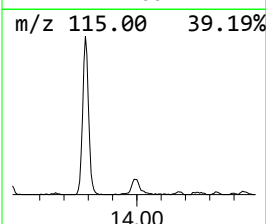
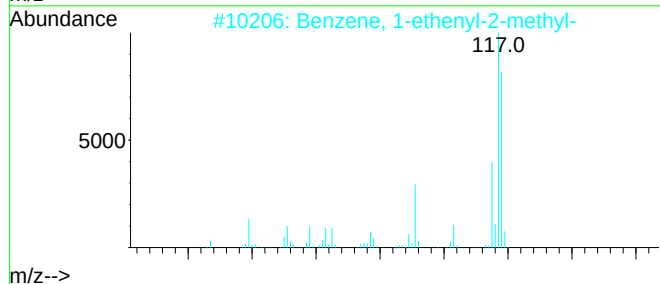
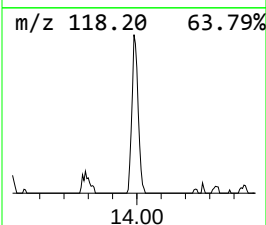
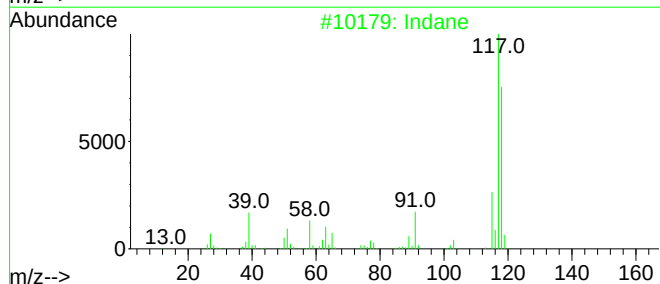
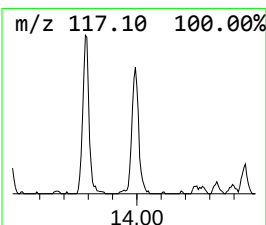
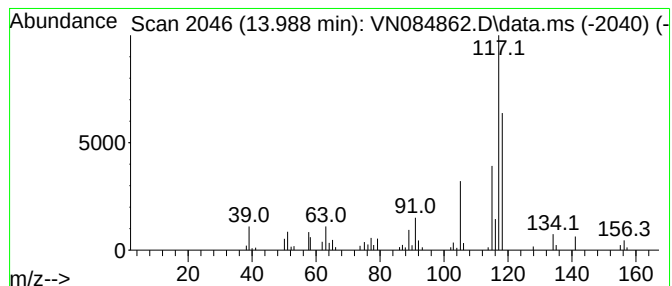
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	10.39 ug/l	199084	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	92
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	58
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	52
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	52
5	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	52



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid	8.753	11.9	ug/l	172683	2	9.100	728016	50.0
Benzene, 1-ethy...	13.094	12.9	ug/l	246331	4	13.788	958185	50.0
Benzene, 1-ethy...	13.335	5.1	ug/l	97275	4	13.788	958185	50.0
Indane	13.988	10.4	ug/l	199084	4	13.788	958185	50.0